Invited Presentation Abstracts

The Impact of In-situ Analysis of Heterogeneous Catalysts for the Improvement of Their Function

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The in-situ analysis of working heterogeneous catalysts has been requested since a long time in the catalysis literature and appears on all strategy planning. It is the inherent complexity of the experiment and the resource-intensive operation of in-situ experiments that still limits the broad application of in-situ techniques both in academia and in industry. A key requirement for efficient operation would be a suitable access to synchrotron radiation facilities with dedicated experiments that form a group of experiments most useful for a large number of catalytic systems.

The contribution will use case studies of molybdate- and vanadate-based catalysts to elucidate the usefulness of in situ studies. This usefulness first is grounded in the access to an understanding of the material science and nanochemistry of such working systems. From there we derive lead ideas for reducing the chemical complexity of novel systems. We identify bottlenecks in our current synthesis strategy for oxide catalysts that are inadequate to obtain the optimal function from materials with a given chemical composition.

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The Hydrogen Economy: Opportunities for Fundamental Research to Address some Grand Challenges

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Abstract

One of the Grand Challenges of the 21st Century is to achieve a sustainable energy supply. The 20th Century has seen remarkable advances in science and technology, resulting in expectations for a higher standard of living. This has required large increases in per capita energy. Projections of per capita energy needs for the 21st Century indicate that new technologies for sustainable energy production, storage, and use will need to be developed in the next 50 years. The so-called hydrogen economy is one such proposal that is presently being considered worldwide and was highlighted in President Bush's 2003 State of the Union Address. In this presentation the requirements of a hydrogen economy will be discussed in the context of the recent DOE report on "Basic Research Needs for the Hydrogen Economy". Hydrogen production, storage and utilization will be discussed with emphasis given to the large gap between present science/technology know-how and the requirements in efficiency/cost for a sustainable hydrogen economy. Opportunities for fundamental research in chemistry and materials to narrow this gap will be discussed.

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DISCOVERY, DEVELOPMENT, AND APPLICATION OF CATALYSTS FOR THE SYNTHESIS OF DEFINED POLYMER ARCHITECTURES, Geoffrey W. Coates, Department of Chemistry and Chemical Biology, Cornell University, Baker Laboratory, Ithaca, New York 14853, gc39@cornell.edu

Single-site polymerization catalysts are molecular complexes with the general formula L_nMR, where L_n is an organic ligand set that remains bound to and thus modifies the reactivity of the active metal center (M) during the entire chemical reaction, and R is an initiating group. By tailoring the coordination environment of the metal center, single-site catalysts are now available that can control the molecular weight, molecular weight distribution, comonomer incorporation, and both the relative and absolute stereochemistry of a polymer in a way that is often not possible using conventional heterogeneous catalysts. The discovery, optimization, and application of several single-site catalysts for the synthesis of polyesters, polyolefins, and polycarbonates will be presented.

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COMPUTER MODELLING AS A TOOL IN CATALYTIC SCIENCE

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Computer modelling techniques are now well established in the study of catalysis at the molecular level, where they are able to provide increasingly accurate and reliable information on active site structures, reaction mechanisms and on the transport of reactants and products to and from the active site. This talk will attempt to review some recent developments in the field by focussing on a number of topical applications, concerning:

i) The mechanisms of epoxidation in metal substituted microporous catalysts, where we will show how joint computational / experimental studies have developed detailed models for active site structures and epoxidation mechanisms.

ii) The mechanisms of methanol synthesis on the surface of ZnO, where we concentrate on the identification of intermediates in this key reaction.

iii) Reactions of small molecules on metal surfaces, where the focus is the identification of transition states of elementary reactions.

The lecture will consider some of the likely future directions in the field.

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